COMBUSTION RESEARCH FACILITY

SAND2018-11413C

Φ-Sensitivity and ITHR – Key Fuel Properties for Advanced Compression Ignition Engines

John E. Dec,
Dario Lopez-Pintor and Gerald Gentz
Sandia National Laboratories

SAE Co-Optimization of Fuels and Engines Symposium
Plymouth, MI – October 9 - 10, 2018

Sponsor:
U.S. DOE, Office of Vehicle Technologies
Program Managers: Gurpreet Singh, Kevin Stork, and Michael Weismiller

Sandia National Laboratories is a multimission laboratory managed and operated by National Technology & Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.

Motivation

- Φ-Sensitivity is a fuel property that has important benefits for the operation of Low-T Gasoline Combst. (LTGC) & all kinetically controlled ACI engines.
- Definition ⇒ a fuel is ϕ-sensitive if its autoignition reactivity varies with the fuel/air equivalence ratio (ϕ) ⇒ for the same thermodynamic conditions.
- Benefits are primarily obtained by using Partial Fuel Stratification (PFS).
  ⇒ Early-DI (or premixed) + late-DI fueling or a single-DI with incomplete mixing to create a distribution of ϕs at time of autoignition.
- Three main beneficial effects:
  1) Φ distribution ➔ sequential autoignition ➔ reduces HRR
     ⇒ **Allows higher loads w/o knock or less CA50 retard for higher efficiency.**
  2) Richer regions autoignite faster, which will advance CA50 (50% burn point)
     ⇒ **Allows CA50 to be controlled by varying late-DI timing or fuel-fraction.**
  3) ITHR increases w/ ϕ-sens. ⇒ **increases allowable CA50 retard & robustness.**

- Φ-sensitivity offers significant benefits, but its chemistry not well understood.
- It would be beneficial to increase ϕ-sensitivity above that of Regular-E10 (RD5-87), particularly at naturally aspirated and low-boost conditions.
- Critical that RON & Octane-Sens. remain high for high loads & SI engines.

Outline

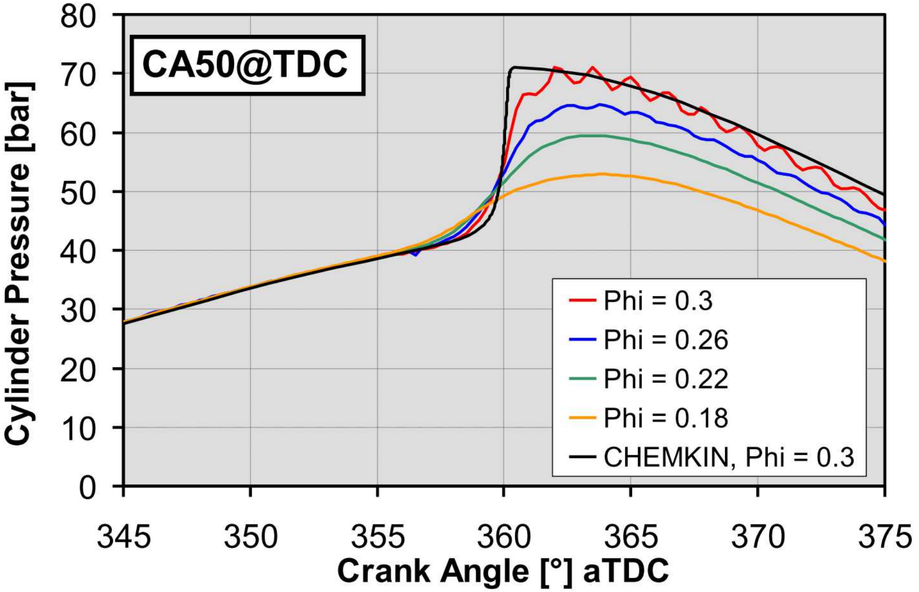
1) Background – Brief explanation of the advantages of charge stratification and the maximum load.
2) Explain ϕ-sensitivity and how it can be combined with controlled fuel stratification to reduce the HRR.
   $\Rightarrow$ Allows higher efficiencies and increased load.
3) Show how PFS with ϕ-sensitive fuels can be used to provide rapid control of combustion timing (CA50).
4) Discuss the advantages of the increased Intermediate Temperature Heat Release (ITHR) associated with ϕ-sensitivity.
5) Investigation of the chemistry of ϕ-sensitivity, using perfectly stirred reactor (PSR) CHEMKIN simulations.
6) Tailoring fuel blends for increased ϕ-sensitivity with higher RON and Octane-sensitivity vs. RD5-87, using CHEMKIN simulations under engine-like conditions.

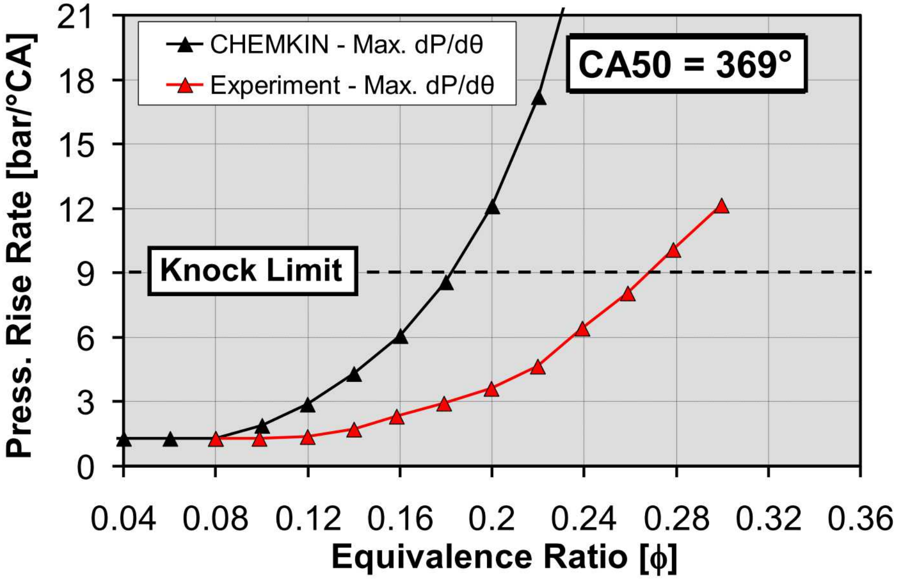
- Co-Optimization: Is it possible to have both high ϕ-sensitivity and high RON with good Octane-sensitivity? $\Rightarrow$ Advantageous for multi-mode engine.

Some Reactivity Stratification is Required for LTGC

- Increased fueling (ϕ) increases pressure-rise rate (PRR), eventually causing knock.
  - **Ringing intensity (RI) = 5 [MW/m²]**, J. Eng, SAE 2002-01-2859.
- CHEMKIN simulation shows effect of fully homogeneous charge.
  - Difference is natural thermal strat.
- This stratification causes autoignition to occur sequentially reducing PRR.
- Retarding CA50 amplifies effect of natural thermal stratification reducing PRR for higher loads w/o knock.
  - Eventually reach retard limit ⇒ poor combust. stability & misfire
  - Retard also reduces thermal efficiency.
- Load limited by knock/stability limit
  - If fueling increased starts to knock
  - Can't retard further to mitigate knock without stability misfire problems.

Fully Premixed, 1200 rpm, iso-Octane

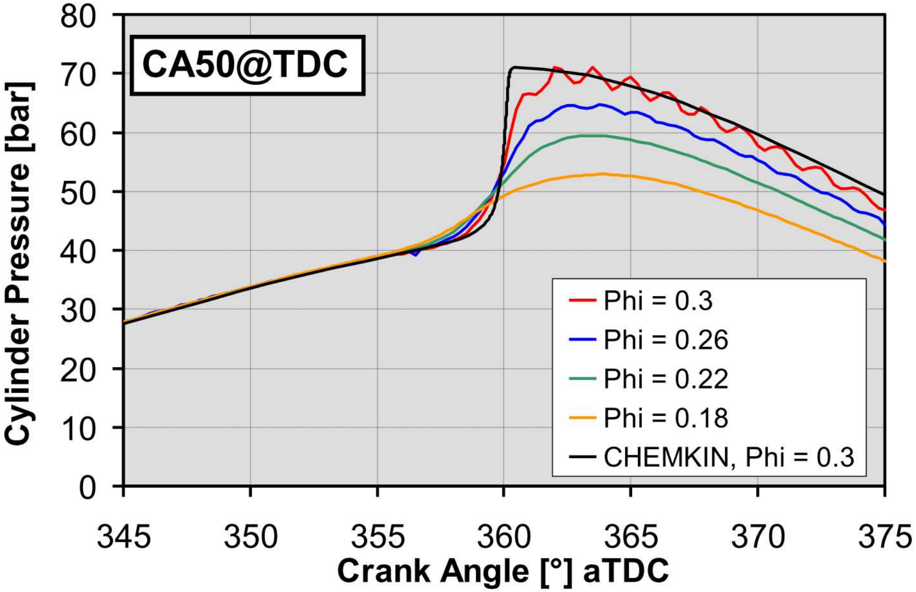


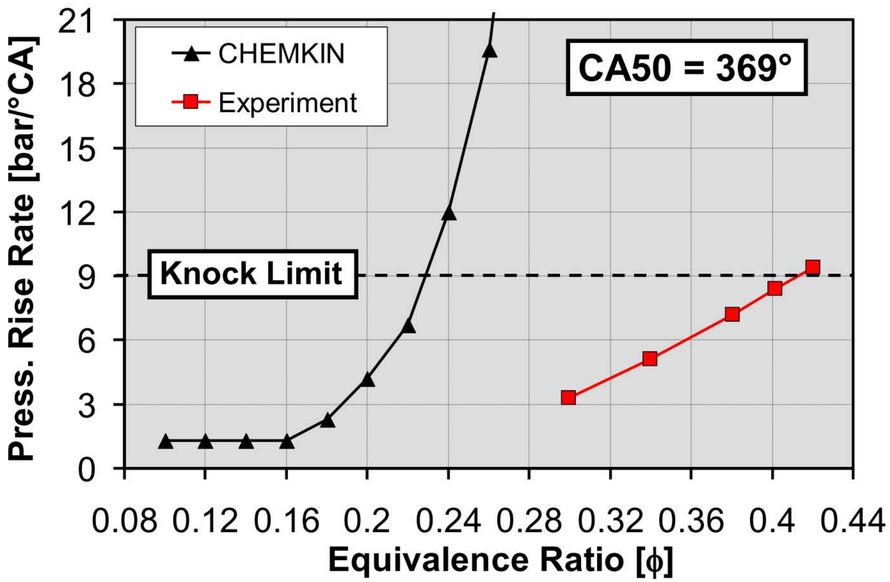


Some Reactivity Stratification is Required for LTGC

- Increased fueling (ϕ) increases pressure-rise rate (PRR), eventually causing knock.
  - **Ringing intensity (RI) = 5 [MW/m²]**, J. Eng, SAE 2002-01-2859.
- CHEMKIN simulation shows effect of fully homogeneous charge.
  - Difference is natural thermal strat.
- This stratification causes autoignition to occur sequentially reducing PRR.
- Retarding CA50 amplifies effect of natural thermal stratification reducing PRR for higher loads w/o knock.
  - Eventually reach retard limit ⇒ poor combust. stability & misfire
  - Retard also reduces thermal efficiency.
- Load limited by knock/stability limit
  - If fueling increased starts to knock
  - Can't retard further to mitigate knock without stability misfire problems.

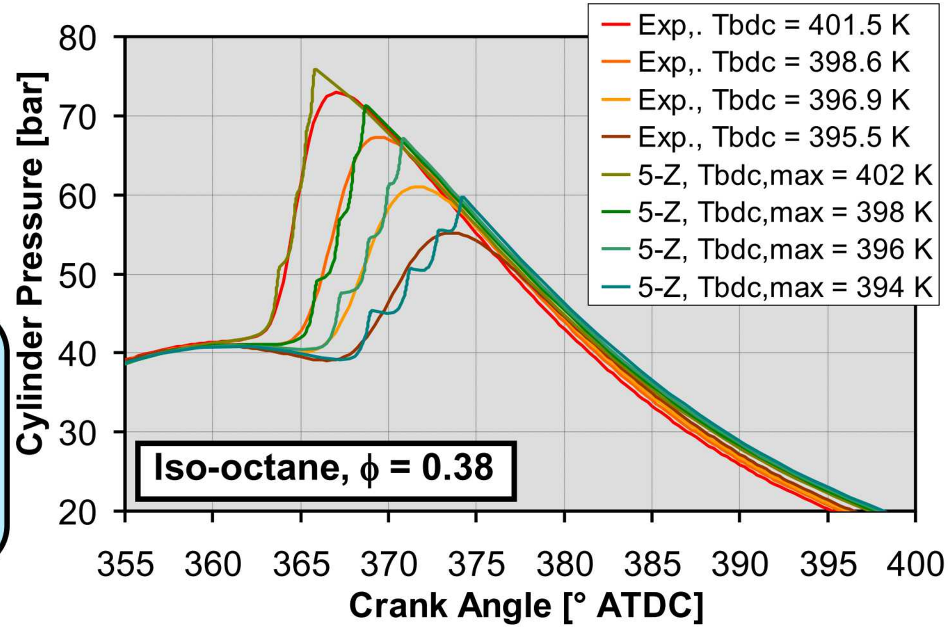
Fully Premixed, 1200 rpm, iso-Octane

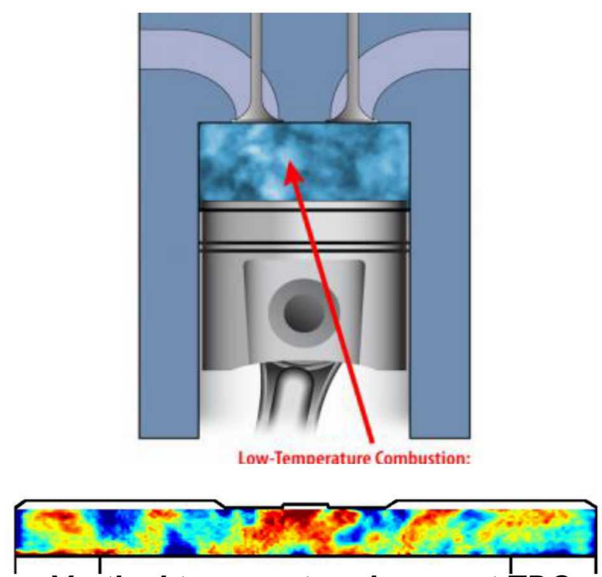




Timing Retard and Sequential Autoignition

- Retarding CA50 reduces HRR & PRR
- Multi-zone CHEMKIN shows that this is due to greater time-delay for sequential autoig. between zones.
- Retarded timing amplifies the benefit of a given stratification.
  ⇒ Allows higher loads w/o knock.
  ⇒ But CA50 retard limited by stability.
- Further load increases require more stratification ⇒ difficult to increase thermal strat. w/o heat loss ↗.
- Mixture stratification can be readily controlled by fuel injection process.
- Can mixture stratification produce sequential autoignition similar to thermal stratification?
- Can we exploit it for higher loads and/or less CA50 retard for TE ↗

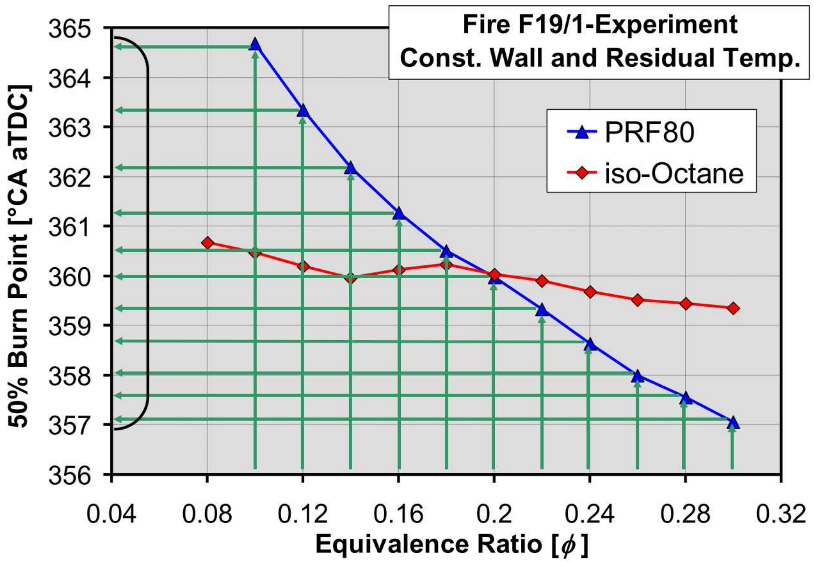


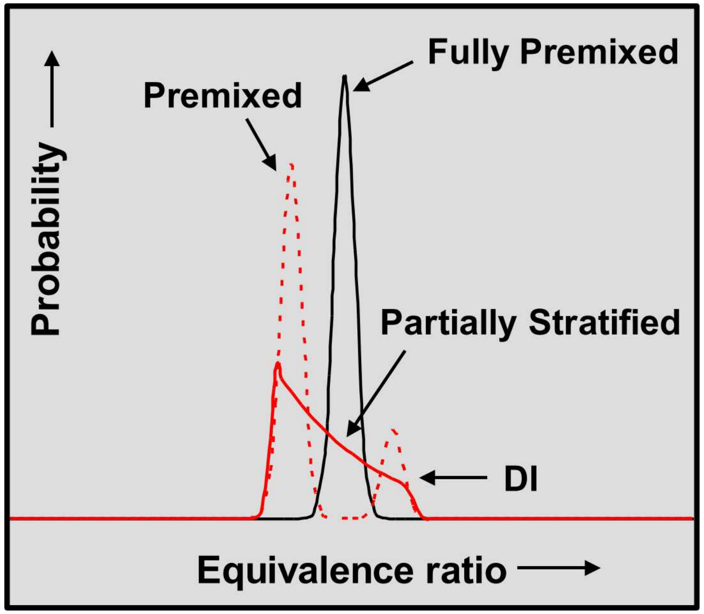


Vertical temperature image at TDC

Controlling the HRR with Partial Fuel Stratification (PFS)

- PFS is effective for controlling HRR and/or CA50, but has two requirements:
  1) Fuel autoig. must be ϕ-sensitive 2) Appropriate ϕ-distribution





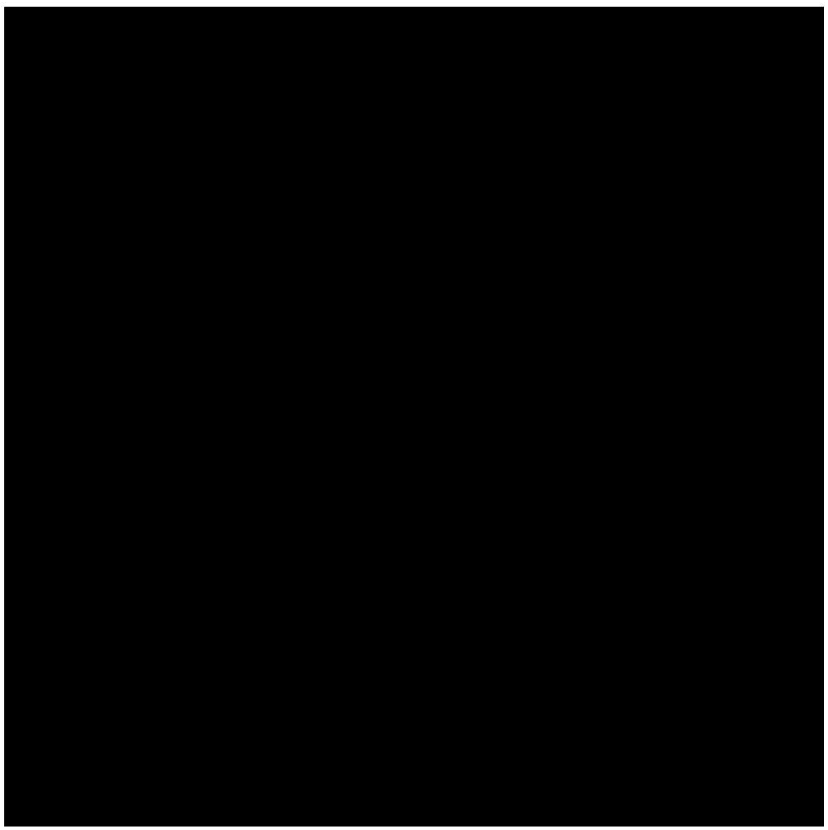
- PRF80 is strongly ϕ-sensitive (2-stage ig.), iso-octane or gasoline is not (1-stage-ig.)
- For ϕ-sensitive fuel, stratifying charge produces sequential autoignition slows HR. ⇒ Higher loads and/or less CA50 retard for higher efficiency.
- **Std. PFS:** most fuel premixed, up to 30% late DI
  - Good air utilization with leanest regions burning hot enough for good combst.
- Other fuel-injection strategies can also be used.

High-Speed Movies (14.4 kHz, 0.5°CA)

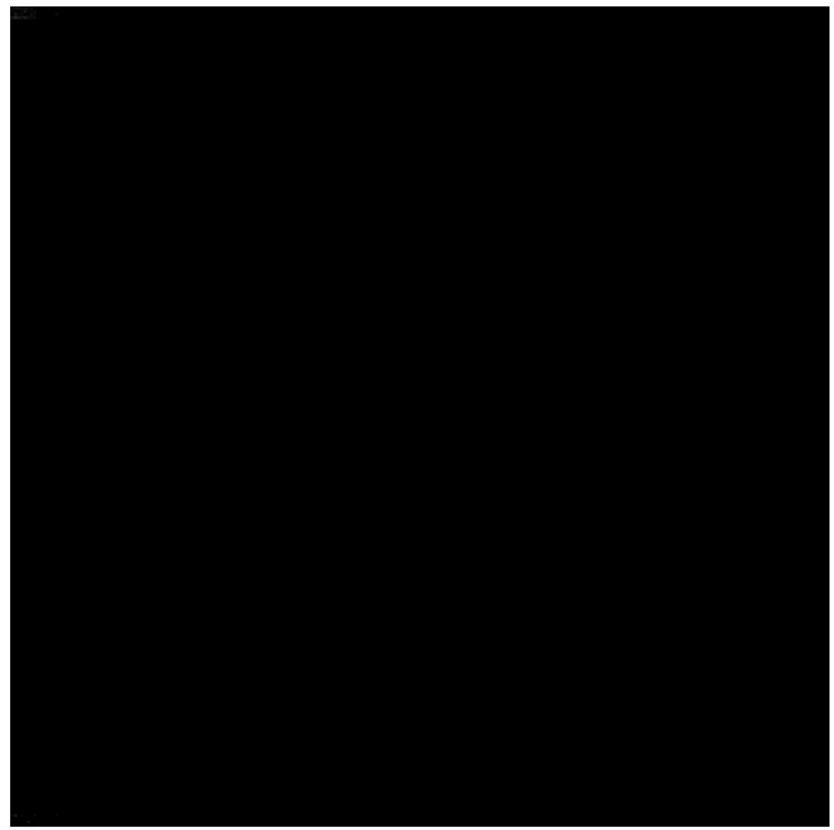
- Both movies show sequential autoignition (PRF80, ϕ = 0.43, P_{in} = 1 bar):
  - Well-mixed: thermal stratification only: combustion relatively rapid.
  - Fuel stratified: ignition spreads from richest $\Rightarrow$ leaner zones: much slower.
- Source of persistent luminosity unclear. Diffusion comb.? But low NO_X and no smoke, metal engine.

ϕ = 0.43

Well Mixed

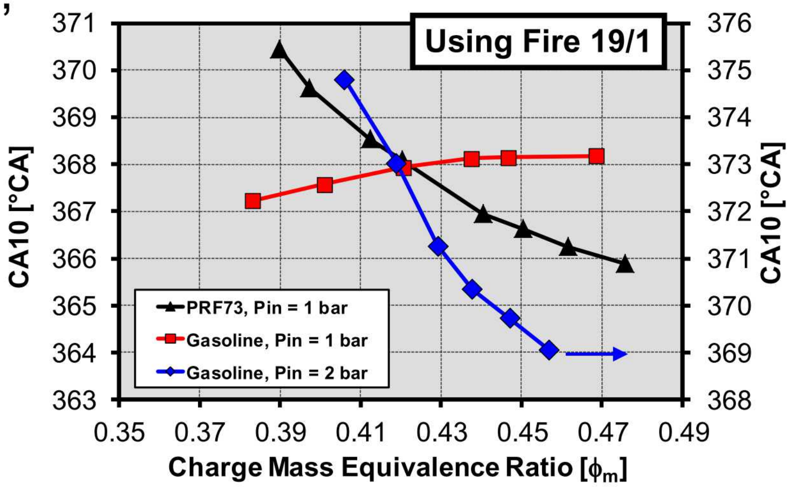


Partial Fuel Stratification with 81% premixed & 19% @ 285°CA

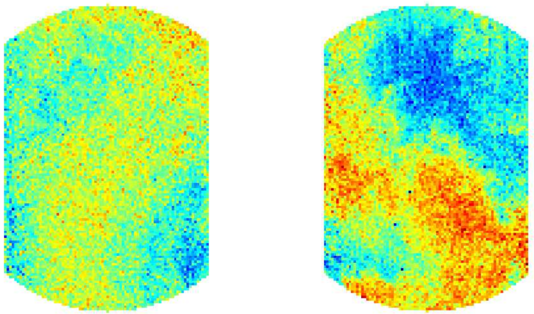


Φ-Sensitivity and PFS of Gasoline

- Previous results show that PFS is effective for controlling HRR for 2-stage ignition fuels like PRF80 at P_{in} = 1.0 bar (naturally aspirated).
- Tests with gasoline show that like iso-octane, it is not ϕ-sensitive for P_{in} = 1.0 bar.
- However, gasoline becomes ϕ-sensitive with boost, and by P_{in} = 2.0 bar, it is more ϕ-sensitive than PRF 73.
- Interestingly, it often doesn't show 2-stage ignition. No LTHR, only enhanced ITHR.
  $\Rightarrow$ ϕ-sensitivity correlates with ITHR
  $\Rightarrow$ will be discussed later.



PLIF images of fuel at 320°CA



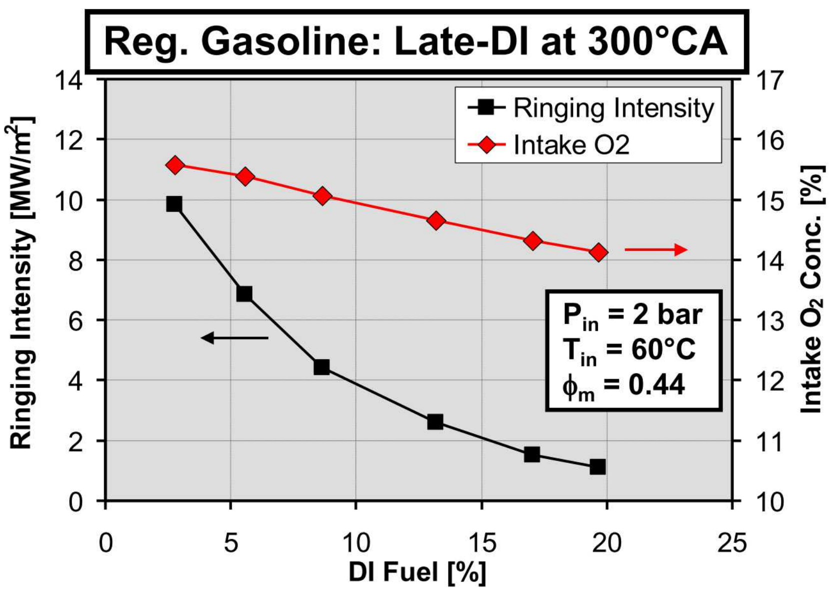
<u>**Premixed**</u> <u>**Early-DI**</u>

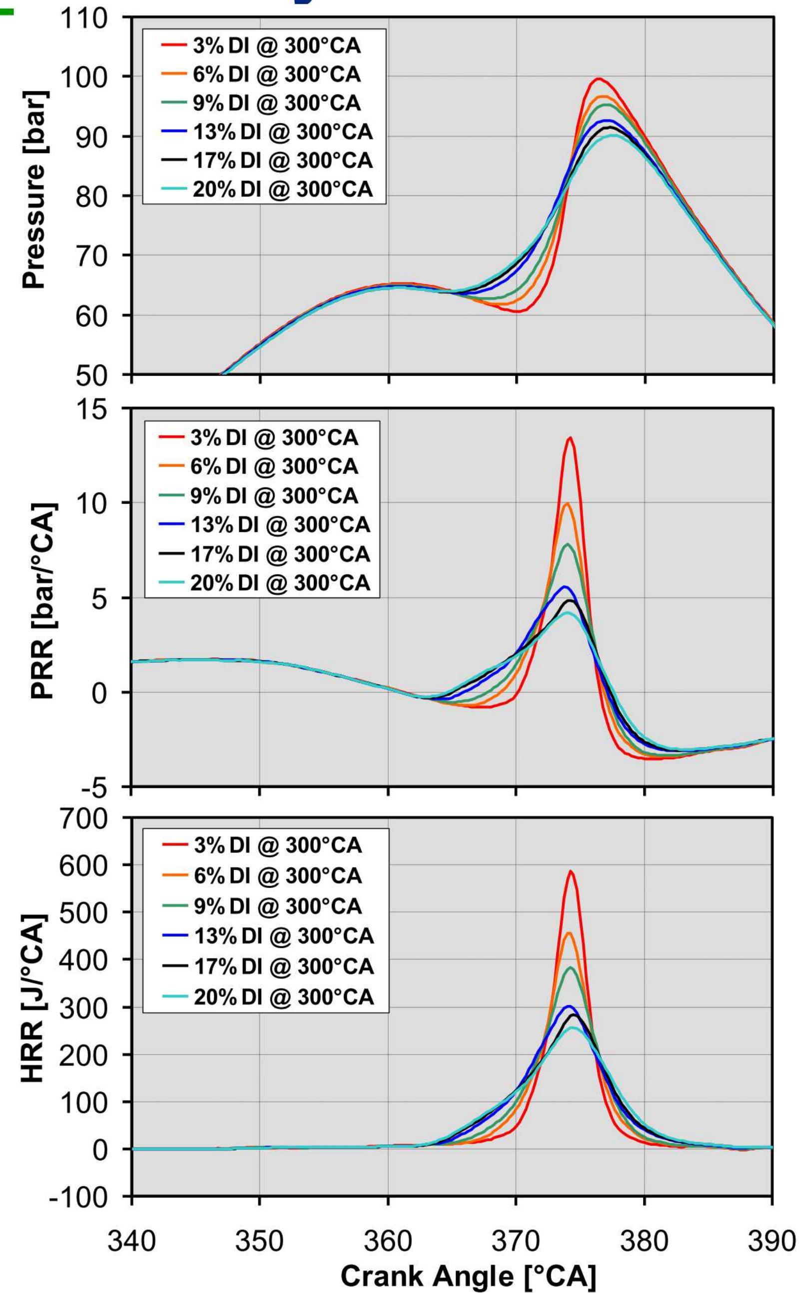
<u>Injection Strategies:</u>

- **Std. PFS:** premix 70-90% + late-DI, $T_{in} \geq 60°C$
- **Early-DI PFS:** inject all fuel at 60°CA
  - Images show not completely mixed.
  - Allows $\mathbf{T_{in} \geq 30°C}$ $\Rightarrow$ high ρ, less EGR, higher γ, and less heat transfer (HT) loss.
- **DDI-PFS:** E-DI 60-90% + late-DI ($T_{in} \geq 30°C$)

Gasoline, P_{in} = 2 bar: Φ-Sensitivity Allows PFS to Greatly Reduce HRR

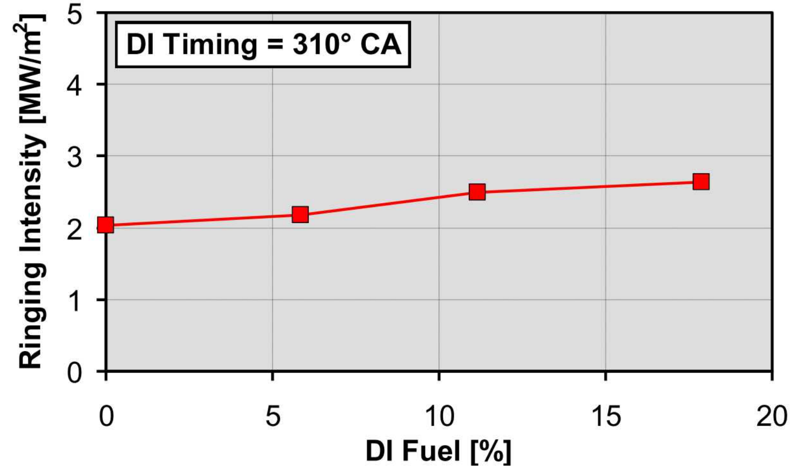
- Std. PFS with late-DI at 300°CA: increasing late-DI% greatly decreases RI & PRR_{max}
- Increases regions of higher $\phi_m \Rightarrow$ autoignite faster $\Rightarrow$ advances hot ignition for same CA50 $\Rightarrow$ increases burn duration
  - Reduces peak HRR, PRR_{max}, and P_{max}. $\Rightarrow$ greatly reduces combustion noise
  - Allows higher loads or adv. CA50 w/o knock.
- Hold CA50 = 374°CA by increasing EGR $\Rightarrow$ Otherwise faster autoignition of richer regions would advance CA50 $\Rightarrow$ timing ctrl.



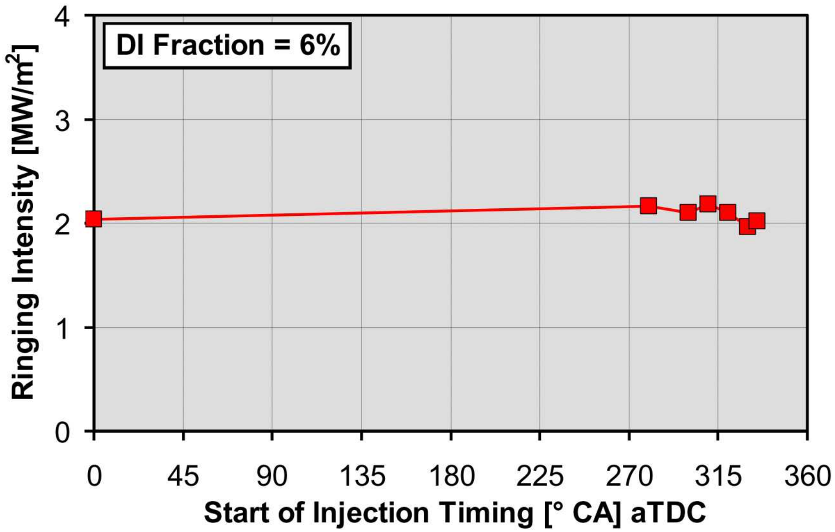


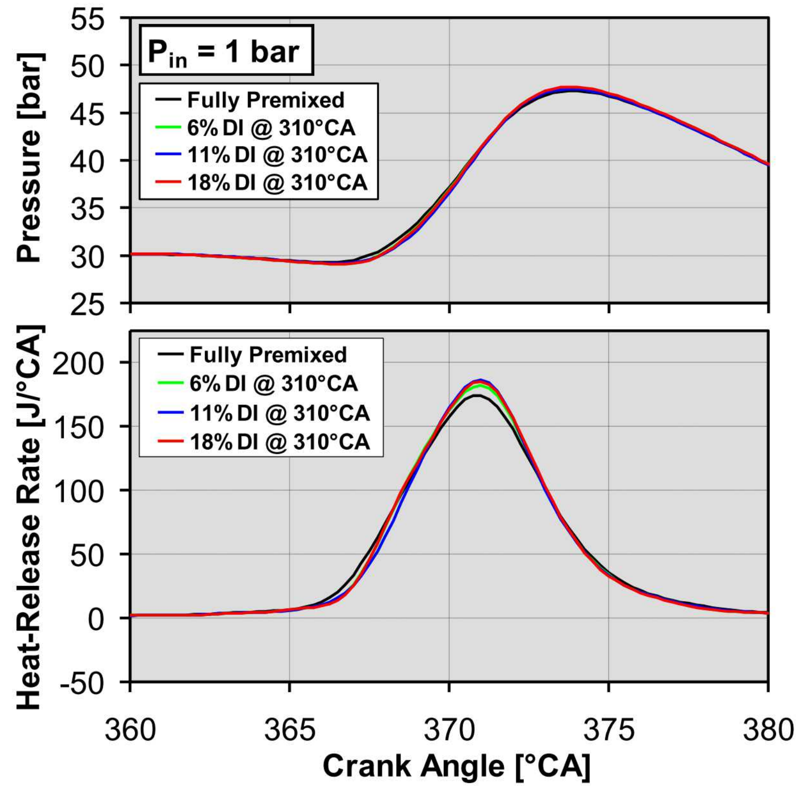
Gasoline, P_{in} = 1 bar: Not Φ-Sensitive, Benefits of PHS Cannot be Realized

- Vary DI timing for const. 6% DI fueling.
  - Ringing & PRR_{max} ~ constant.
- Increase DI fraction; SOI = 310°CA.
  - Ringing increases slightly.
- Gasoline at P_{in} = 1 bar ⇒ PFS has no benefit for reducing HRR & PRR_{max} for the these levels of stratification.
  - Agrees with low ϕ-sensitivity for $\phi \leq 0.47$ shown in previous slide.



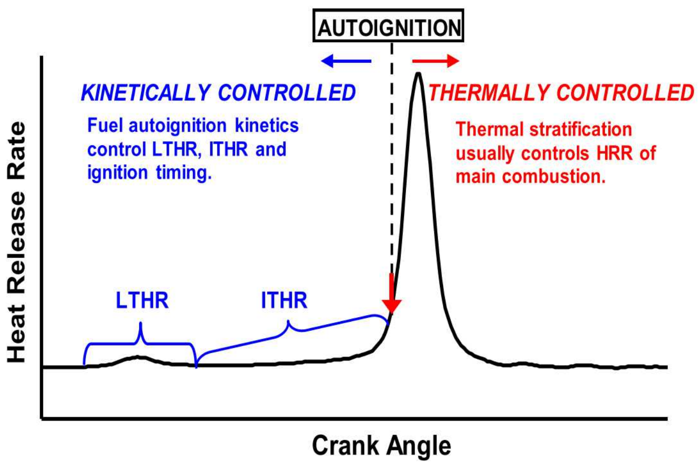
Gasoline: hold CA50 = 371°CA, ϕ_m = 0.44, T_{in} ~ 143°C

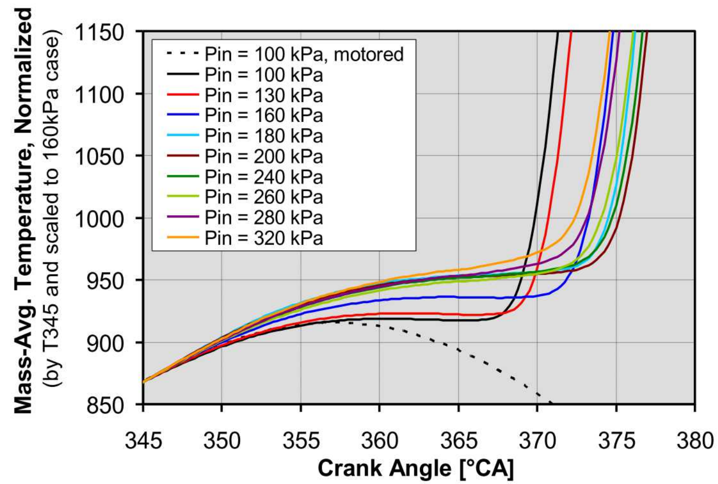


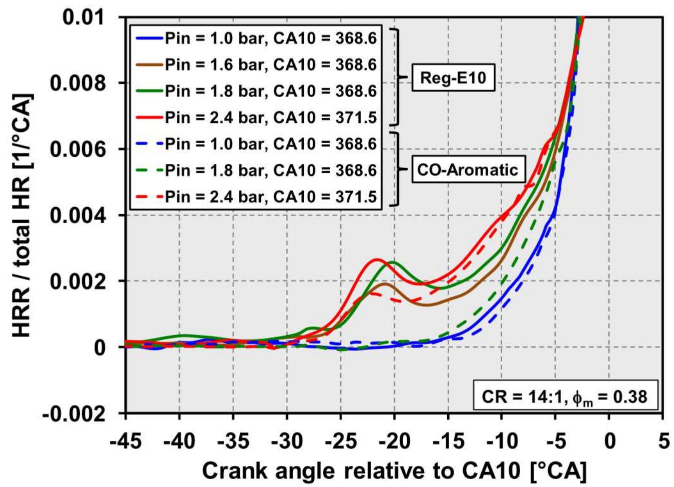


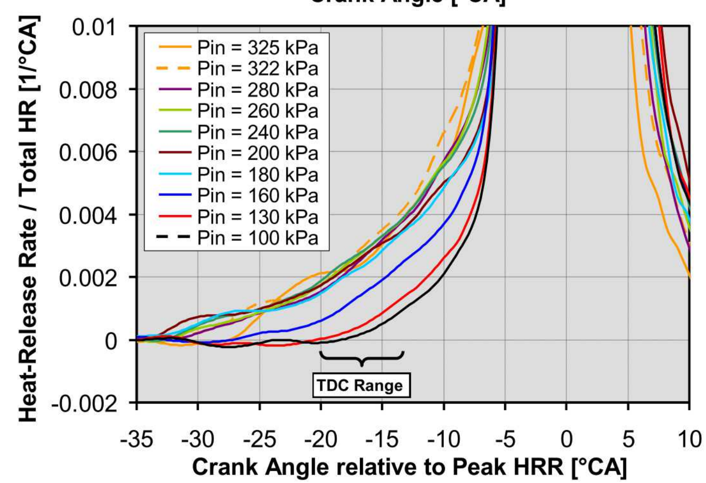
Φ-Sensitivity Correlates with ITHR

- Experiments show ⇒ amount of Intermediate-Temperature Heat Release (ITHR) increases for fuels or operating conds. that have increased ϕ-sensitivity.
  - Conversely, amount of ITHR can be used to predict ϕ-sensitivity.
- Stronger ITHR also allows more CA50 retard w/ good stability ⇨ keeps T rising.
  - Provides benefits even for premixed operation.



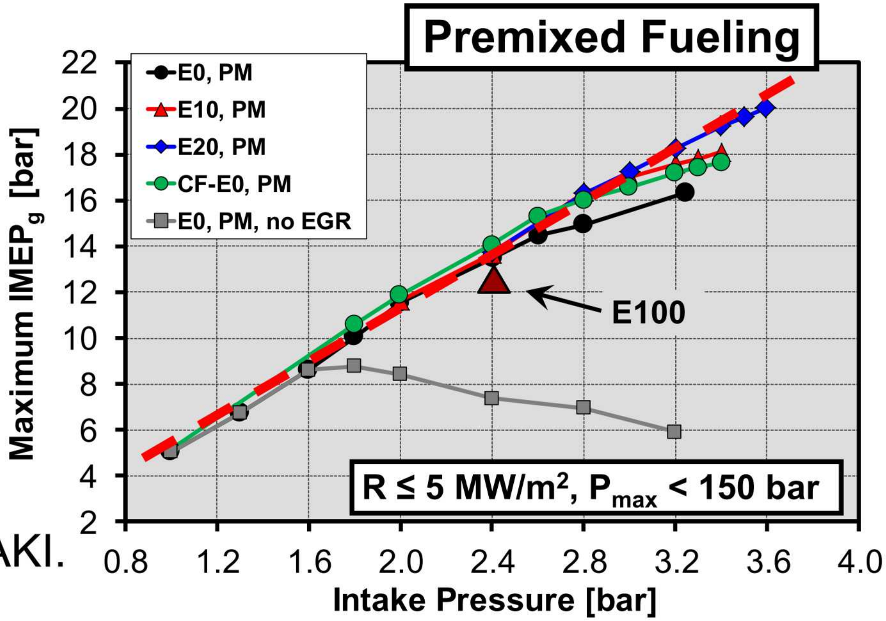


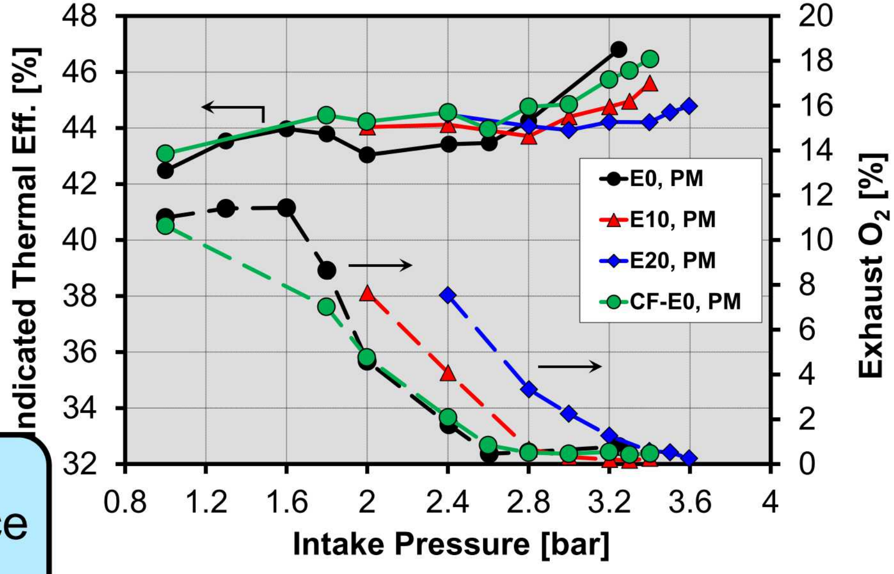




Increased ITHR Allows Large Load Increase with Boost for Premixed Fueling

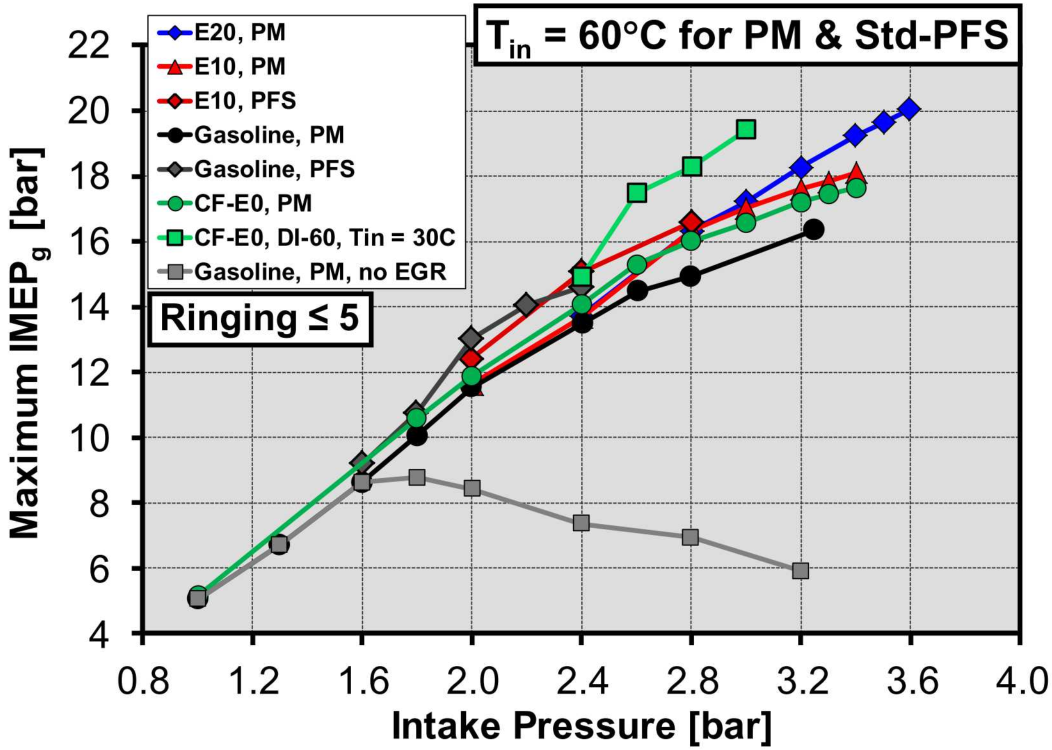
- ITHR ↗ with boost allows more CA50 retard with good stability ⇒ higher loads.
- Gasoline reactivity increases w/ boost.
  - Use EGR to control CA50.
  - Eventually, EGR ↗ limits O_2 for combst.
- Reduce fuel reactivity to reduce EGR ⇒ E0, 87 AKI ⇒ E10, 90.5 AKI ⇒ E20, 93 AKI, and Tier II CF, 93 AKI
  - Tier II CF more reactive than E20, same AKI.
- Achieved 20 bar $IMEP_g$, but P_{in} = 3.6 bar.
  - Load ↗ w/ boost becomes almost linear.
  - Reduced reactivity does not increase load above line.
- Further reducing reactivity can reduce ITHR ⇒ lower stability ⇒ lower max. load.
  - E100 has no ITHR ↗ w/ boost ⇒ load↘
- Increasing load above line requires higher fueling rate at a given boost. ⇒ Must reduce HRR w/o increasing CA50 retard.





PFS Increases Load-to-Boost Ratio

- PFS fueling reduces PRR_{max} ⇒ allows higher loads with less CA50 retard
  - Std.-PFS increases Max. Load at intermediate boost (T_{in} = 60°C).
    - No increase at higher P_{in} because O_2 limited.
  - Early-DI PFS allows T_{in} = 30°C ⇒ less EGR required (> O_2), more charge mass.
    - Substantial increase in Max. Load for P_{in} ≥ 2.4 bar.



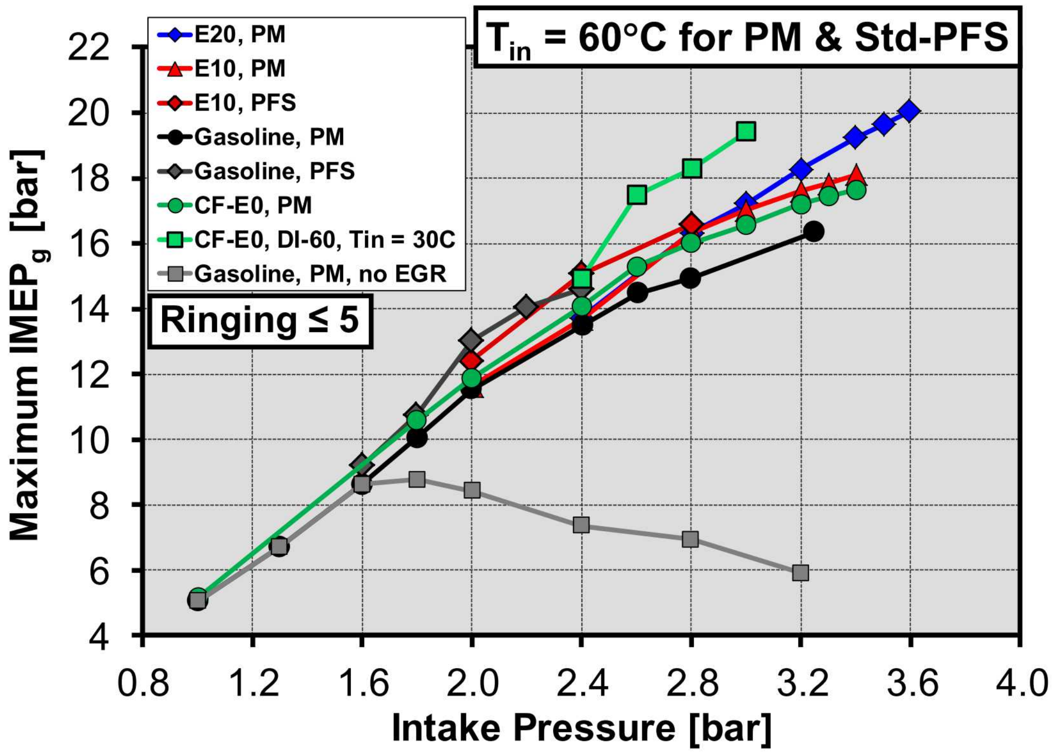
Max. loads limited by cylinder-head pressure limit

For all boosted data, NO_X ≤ 10% of US 2010 and Smoke is not detectable.

- **Early-DI PFS ⇒ 19.4 bar $IMEP_g$ for P_{in} = 3 bar**

PFS Increases Load-to-Boost Ratio

- PFS fueling reduces PRR_{max} ⇒ allows higher loads with less CA50 retard
  - Std.-PFS increases Max. Load at intermediate boost (T_{in} = 60°C).
    - No increase at higher P_{in} because O_2 limited.
  - Early-DI PFS allows T_{in} = 30°C ⇒ less EGR required (> O_2), more charge mass.
    - Substantial increase in Max. Load for P_{in} ≥ 2.4 bar.



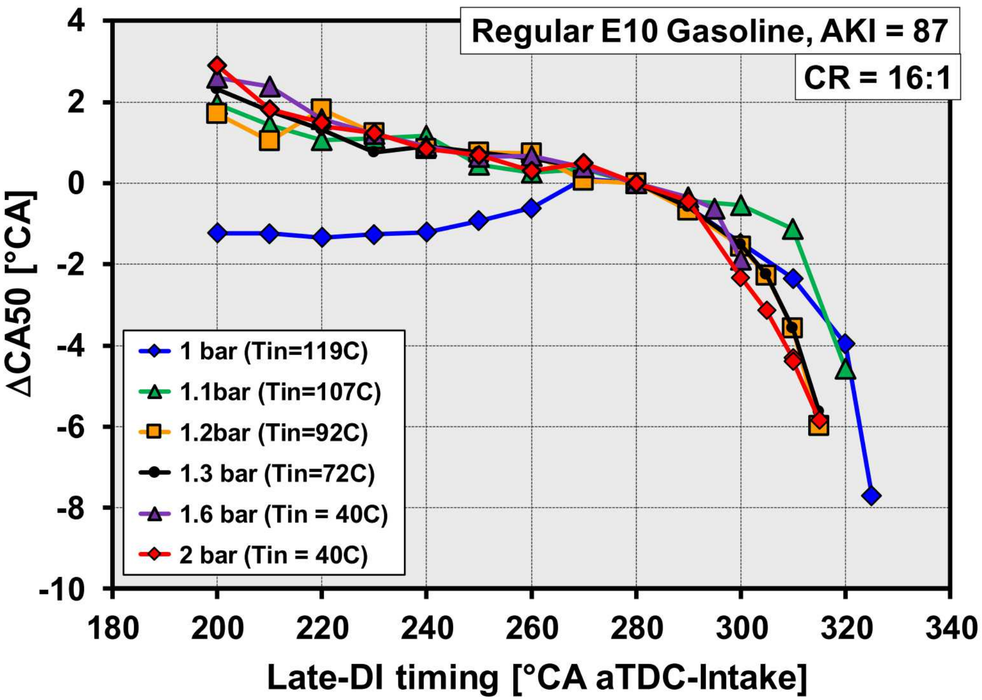
Max. loads limited by cylinder-head pressure limit

For all boosted data, NO_X ≤ 10% of US 2010 and Smoke is not detectable.

- **Early-DI PFS ⇒ 19.4 bar $IMEP_g$ for P_{in} = 3 bar ⇒ Load-to-boost ratio similar to diesel engines. ⇒ Load exceeds production diesel version of engine ~19 bar.**

Φ-Sens. allows CA50 control by varying PFS

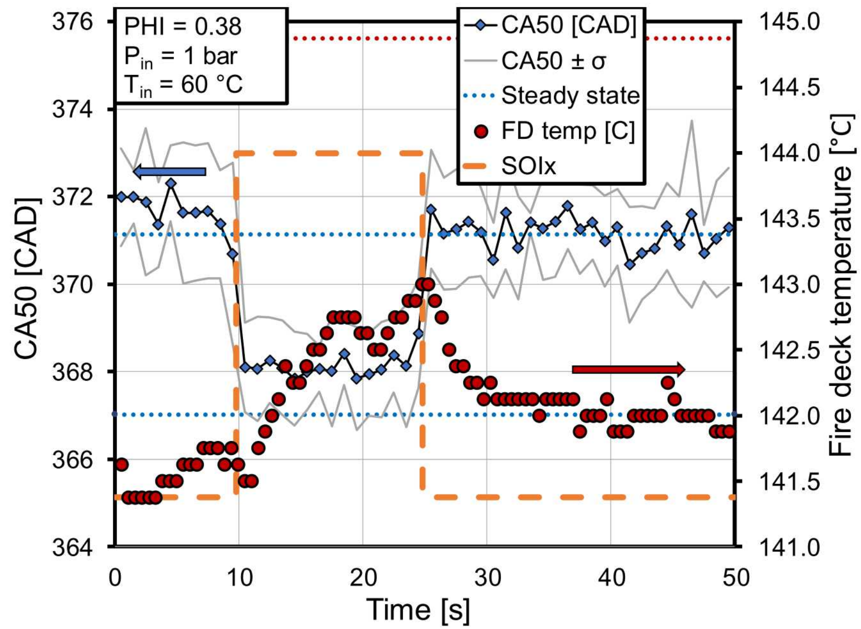
- For ϕ-sensitive fuels w/ PFS, richer regions autoignite faster, advancing CA50. ⇒ Control CA50 by varying the stratification using DDI-PFS.
- 2nd-DI timing of 200° CA ⇒ fairly well-mixed ⇒ CA50 is quite retarded.
- Increase stratification by delaying 2nd-DI timing ⇒ increases the ϕs of the richest regions ⇒ advances CA50.
- Curves are similar for all P_{in}s from 2.0 to 1.2 bar ⇒ sufficient ϕ-sensitivity.
  - For P_{in} = 1.1 bar, more stratification (later 2nd-DI timing) is required as ϕ-sensitivity decreases.
  - P_{in} = 1.0 bar, fuel is less ϕ-sensitive ⇒ little effect until 2nd-DI timing ≥ 270° CA ⇒ good CA50 control possible with this greater stratification.

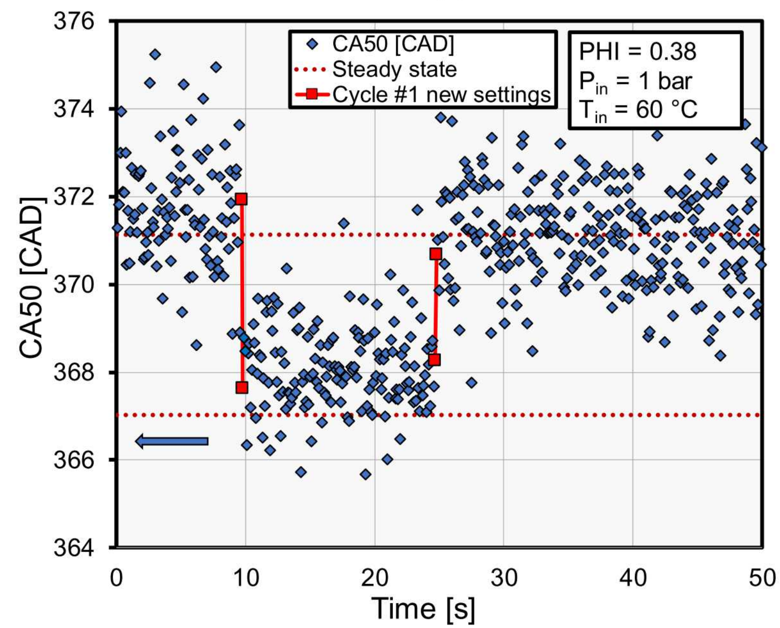


- For a fuel with the ϕ-sensitivity of RD5-87, PFS can give 6.5 – 8.5°CA of control authority for P_{in}= 1 – 2 bar.
- Increasing the fuel's ϕ-sensitivity would likely provide greater control authority & more robustness.

PFS Can Provide Next-Cycle CA50 Control

- Example demonstrates CA50 advancement by changing PFS and return to original setting 15 secs. later.
- **PFS changes CA50 from one cycle to the next.**
- Interestingly, the advanced CA50 does not reach equilibrium value ⇒ because T_{wall} only shifts halfway to equilibrium temperature in 15 seconds.
- Control system must overdrive CA50 change, then adjust back as walls warm up.



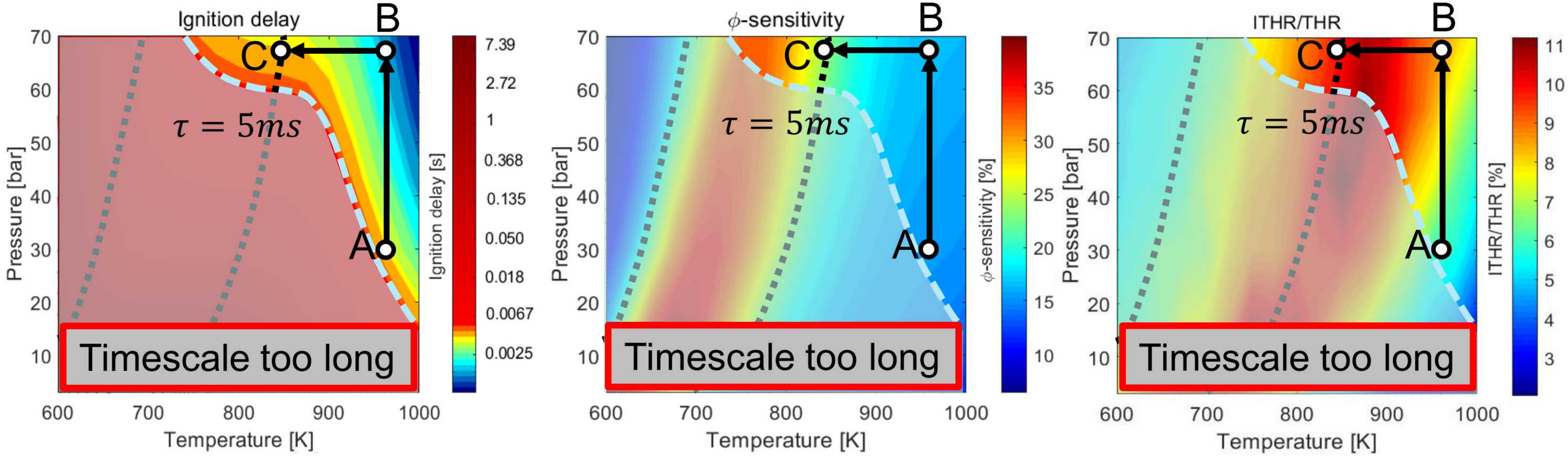


Understanding Φ-Sensitivity and ITHR

- Φ-sensitivity offers many benefits for LTGC and other kinetically controlled (KC) ACI combustion methods, including mixed-mode operation.
  - Experimentally observed that Φ-sensitivity is associated with an increase in ITHR, which is also beneficial for LTGC / KC-ACI.
  - The amounts of Φ-sensitivity and LTHR vary with operating condition and fuel composition.
- Increasing the Φ-sensitivity and ITHR offers substantial benefits for LTGC / KC-ACI.
  ⇒ Particularly, at P_{in} = 1.0 – 1.6 bar where these effects are weaker and where mixed-mode engines typically operate in LTGC-mode.
- Can these properties be enhanced while maintaining or increasing RON and octane sensitivity, which are advantageous for boosted-SI operation?
- Apply CHEMKIN chemical-kinetics calculations using LLNL detailed mech.
  1. Understand the source of Φ-sensitivity and it's relationship to ITHR.
  2. Investigate the potential of developing fuel blends that have enhanced Φ-sensitivity and ITHR, but still have high RON and octane-sensitivity.

Investigate Φ-Sensitivity & ITHR, and their Relationship to Octane Sensitivity

- Φ-Sensitive fuels allow controlled charge stratification to provide CA50 control, load extension, and noise reduction ⇒ <u>Chemical-kinetics of Φ-sensitivity not understood.</u>
- Applied CHEMKIN with detailed mechanism
  - Select iso-octane as a representative fuel with NTC behavior (Φ_m = 0.4, 21% O2).

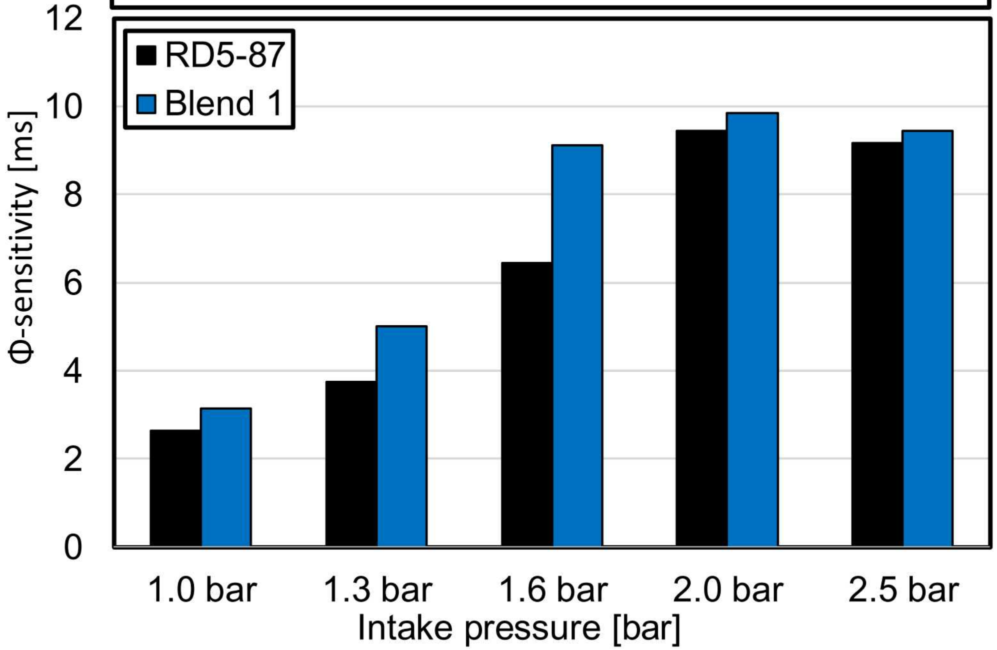


- Φ-Sensitivity is greatest in the **NTC zone ⇒ but still significant on the edges.**
- Intermediate temp. heat release (ITHR) has same trend, but offset to higher Temps. ⇒ **The ITHR chain branching reactions control the Φ-sensitivity.**
- For gasoline-like fuels at P_{in} = 1.0 bar, usually T > NTC zone ⇒ With boost, T must be reduced, both P➚ & T➘ shift operation toward NTC zone, increasing ϕ-sensitivity.
- Is it possible to have a fuel w/ increased Φ-sens. at low P_{in} and high RON & high S?

Explore the Potential to Increase Both Φ-Sensitivity & Octane Sensitivity Above Reg-E10 (RD5-87)

- CHEMKIN simulations with detailed mechanism ⇒ Φ-sensitivity = $\frac{d\tau}{d\Phi}[ms]$
- Multiple fuel blends tested using a systematic methodology.
- <u>Best blend without legal limitations:</u>

76.5% 1-hexene + 23.5% p-xylene



EPA limits: Olefins ≤ 17.5%
Aromatics ≤ 30.4%

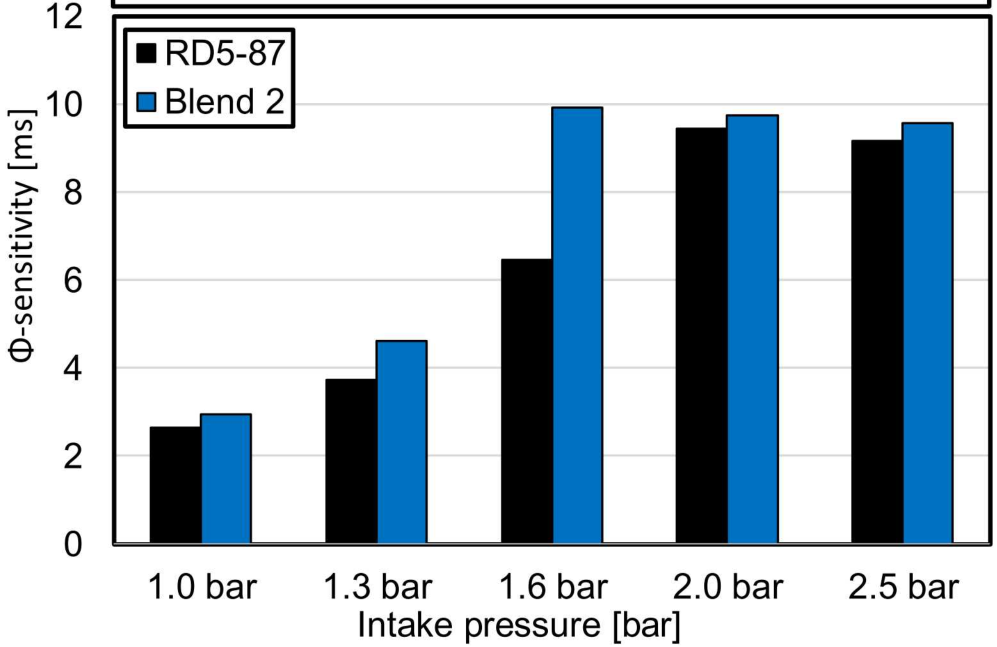
	RON	MON	S	T_{BCD} (1bar)	H/C ratio	O/C ratio
RD5-87	92.1	84.8	7.3	408K	2.025	0.0335
Blend 1	108.4	94	14.4	401.5K	1.782	0

Explore the Potential to Increase Both Φ-Sensitivity & Octane Sensitivity Above Reg-E10 (RD5-87)

- CHEMKIN simulations with detailed mechanism ⇒ Φ-sensitivity = $\frac{d\tau}{d\Phi}[ms]$
- Multiple fuel blends tested using a systematic methodology.
- Best blend that meets EPA regulations:

17.5% 1-hexene + 21% 2-methyl-hexane + + 30% p-xylene + 31.5% iso-octane

EPA limits: Olefins ≤ 17.5%
Aromatics ≤ 30.4%

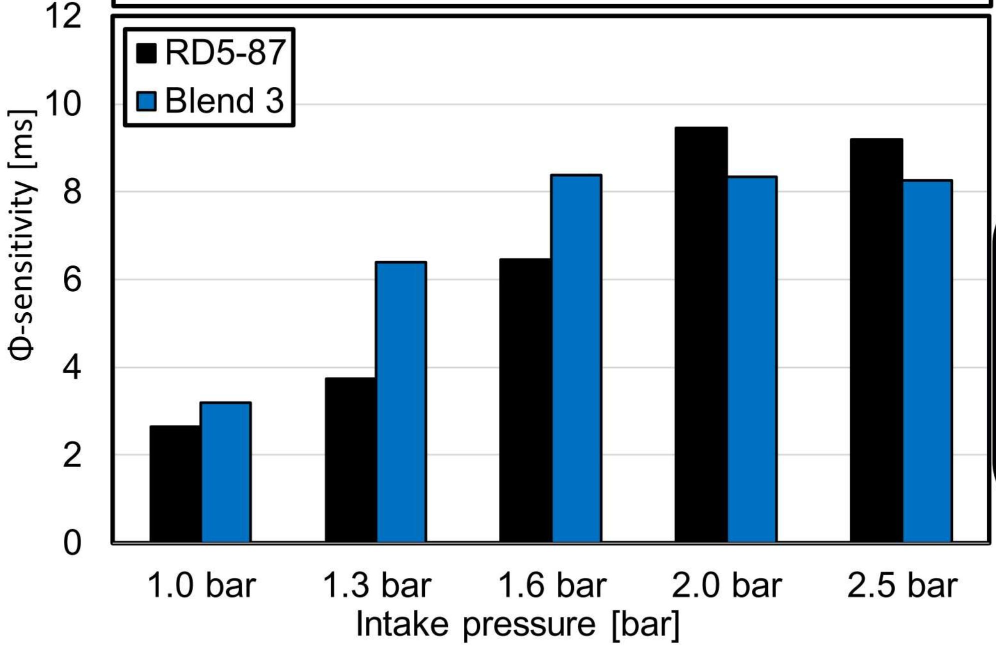


	RON	MON	S	T_{BCD} (1bar)	H/C ratio	O/C ratio
RD5-87	92.1	84.8	7.3	408K	2.025	0.0335
Blend 2	98.5	92.2	6.3	414K	1.899	0

Explore the Potential to Increase Both Φ-Sensitivity & Octane Sensitivity Above Reg-E10 (RD5-87)

- CHEMKIN simulations with detailed mechanism ⇒ Φ-sensitivity = $\frac{d\tau}{d\Phi}[ms]$
- Multiple fuel blends tested using a systematic methodology.
- Best blend that meets EPA regulations and includes a high-performance fuel (HPF):

17.5% 1-hexene + 23.3% 2-methyl-hexane + + 30% p-xylene + 29.2% iso-butanol



EPA limits: Olefins ≤ 17.5%
Aromatics ≤ 30.4%

- All fuels show high Φ-sensitivity at high pressures (P_{in} >1.6 bar)
- Achieved a significant Φ-sensitivity improvement at low & medium press. (P_{in} ≤ 1.6 bar)
- RONs are high, and Ss are good.
  ⇒ Good for boosted-SI or multi-mode
- Iso-butanol and 2-butanol are promising HPF species.

	RON	MON	S	T_{BCD} (1bar)	H/C ratio	O/C ratio
RD5-87	92.1	84.8	7.3	408K	2.025	0.0335
Blend 3	97.6	87.0	10.6	402K	1.880	0.0467

Summary and Conclusions

- Φ-sensitivity combined with PFS provides several benefits for LTGC engine combustion:
  1) Allows higher loads without knock or excessive CA50 retard.
  2) Can increase efficiency because it reduces the required CA50 retard.
  3) Can reduce combustion noise.
  4) Allows the use of multiple fuel injections to control CA50.
- Increased ITHR associated with Φ-sensitivity improves combustion stability and robustness ⇒ particularly valuable for high CA50 retard (and noise reduction).
- Chemical-kinetic calculations show that Φ-sensitivity
  - Results mainly from ITHR chain-branching reactions.
  - Is strongest in the NTC (negative temperature coefficient) region but it is still strong on the edges of these regions.
- Even though Φ-sensitivity is highest in NTC region where octane sensitivity typically low, CHEMKIN calculations show that it is possible to blend a fuel with both high Φ-sensitivity and high octane sensitivity.
  - Computationally demonstrated three blends that increase Φ-sensitivity over base fuel (RD5-87), while increasing RON and octane sensitivity (S).
  - Best fuel was a 29% iso-butanol blend, RON = 97.6, S = 10.6, and significantly higher Φ-sensitivity at low and intermediate boost pressures (P_{in} = 1.0 – 1.6 bar)

Acknowledgement

- This work was performed at the Combustion Research Facility, Sandia National Laboratories, Livermore, CA.

  Sandia National Laboratories is a multi-mission laboratory managed and operated by National Technology and Engineering Solutions of Sandia, LLC, a wholly owned subsidiary of Honeywell International, Inc., for the U.S. Department of Energy's National Nuclear Security Administration under contract DE-NA0003525.